

The Kondo lattice model with correlated conduction electrons

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We investigate a Kondo lattice model with correlated conduction electrons. Within dynamical mean-field theory the model maps onto an impurity model where the host has to be determined self-consistently. This impurity model can be derived from an Anderson-Hubbard model both by equating the low-energy excitations of the impurity and by a canonical transformation. On the level of dynamical mean-field theory this establishes the connection of the two lattice models. The impurity model is studied numerically by an extension of the non-crossing approximation to a two-orbital impurity. We find that with decreasing temperature the conduction electrons first form quasiparticles unaffected by the presence of the lattice of localized spins. Then, reducing the temperature further, the particle-hole symmetric model turns into an insulator. The quasiparticle peak in the one-particle spectral density splits and a gap opens. The size of the gap increases when the correlations of the conduction electrons become stronger. These findings are similar to the behavior of the Anderson-Hubbard model within dynamical mean-field theory and are obtained with much less numerical effort.

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I. INTRODUCTION

The usual explanation for the formation of heavy fermions in compounds with rare-earth or actinide elements is based on the Kondo effect.^{1,2} Thereby, the characteristic low-energy scale arises from the spin-screening of the local moments by a non-interacting electron gas. The periodic Anderson model, as well as the Kondo lattice model, are considered as the most promising candidates to at least qualitatively describe the rich physics of these materials. However, these models fail³ to describe correctly the temperature scale of the heavy-fermion behavior in the electron-doped cuprate $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ discovered a few years ago.⁴ It has therefore been suggested that the strong correlations among the doped carriers which are usually neglected in the Kondo effect play a crucial role and may enhance the Kondo temperature significantly.³ Subsequently, efforts have been undertaken in order to study the influence of the correlations among the conduction electrons on the Kondo effect, both for impurity⁵⁻¹² and lattice¹³⁻¹⁵ models.

These correlations are usually introduced by adding a Hubbard-type interaction among the conduction electrons to the Anderson model. In Ref. 15 the resulting (periodic) Anderson-Hubbard model was investigated within the dynamical mean-field theory.^{16,17} It was shown that it maps onto an impurity model where the impurity consists of a unit cell of the lattice model, i.e., of two correlated orbitals. This model still includes charge fluctuations on the f orbital which should not influence the low-energy behavior in the Kondo limit. It would be desirable to eliminate these degrees of freedom as this reduces the number of states of the impurity and thus reduces the

computational effort to investigate the impurity model. Hence, we are aiming at a Kondo-Hubbard model as the counterpart of the Anderson-Hubbard model just as in the case of uncorrelated conduction electrons.¹⁸⁻²⁰

In the next section, we introduce the Kondo-Hubbard model and map it to an impurity model using the dynamical mean-field approximation. In Sec. III we relate the derived effective impurity model with the one of the Anderson-Hubbard model. We have applied the resolvent perturbation theory²¹ to investigate the effective impurity model for the Kondo-Hubbard model. We present some results in Sec. IV and finally conclude in Sec. V.

II. THE KONDO-HUBBARD MODEL

The (periodic) Kondo-Hubbard model is given by

$$H_K = H_c + H_S, \quad (1)$$

$$H_c = \sum_{k\sigma} \left(\epsilon_k - \frac{1}{2} U_c \right) c_{k\sigma}^\dagger c_{k\sigma} + U_c \sum_i n_{i\uparrow}^c n_{i\downarrow}^c, \quad (2)$$

$$H_S = J \sum_i \vec{S}_i^f \vec{S}_i^c. \quad (3)$$

Here, the c operators refer to the conduction electrons which are described by a Hubbard model with on-site repulsion U_c . $\vec{S}_i^{c(f)}$ denotes the spin of an electron at site i in the conduction band orbital c and the impurity orbital f , respectively. For simplicity we consider in this paper the particle-hole symmetric model only, which implies $\mu = 0$.

We closely follow the treatment of the usual Kondo lattice model in infinite dimensions given in Ref. 22. We introduce Fermion operators $d_{i\sigma}$ to represent the f spin

$$\vec{S}_i^f = \frac{1}{2} \sum_{\sigma\sigma'} d_{i\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} d_{i\sigma'} \quad (4)$$

with local constraints

$$Q_i = \sum_{\sigma} d_{i\sigma}^\dagger d_{i\sigma} = 1 \quad (5)$$

for all i . To enforce the constraints we add

$$H_U = \frac{1}{2} U \sum_i (Q_i - 1)^2 \quad (6)$$

to the Hamiltonian and take the limit $U \rightarrow \infty$.²² The Hamiltonian H_K includes three two-particle parts proportional to J , U_c and U , respectively. Given the non-interacting Green's function, $G_0(\vec{k}, \omega)$, of the Kondo-Hubbard model

$$G_0^{-1}(k, \omega) = \begin{pmatrix} \omega + \frac{1}{2}U_c - \epsilon_k & 0 \\ 0 & \omega + \frac{1}{2}U \end{pmatrix} \quad (7)$$

the self-energies are defined by Dyson's equation

$$G(k, \omega) = (G_0^{-1}(k, \omega) - \Sigma(k, \omega))^{-1}. \quad (8)$$

The dynamical mean-field theory assumes a momentum-independent self-energy matrix²³ $\Sigma(k, \omega) \rightarrow \Sigma(\omega)$ which holds in the limit of infinite dimensions.²⁴ Following the arguments given in Ref. 15 we can calculate $\Sigma(\omega)$ from the impurity model

$$H_{K,\text{imp}} = H_{\text{loc}} + H_{\text{med}}, \quad (9)$$

$$H_{\text{loc}} = -\frac{1}{2}U_c \sum_{\sigma} c_{\sigma}^\dagger c_{\sigma} + U_c n_{\uparrow}^c n_{\downarrow}^c + J \vec{S}^f \vec{S}^c \quad (10)$$

$$H_{\text{med}} = \sum_{k\sigma} E_k \alpha_{k\sigma}^\dagger \alpha_{k\sigma} + \sum_{k\sigma} \left(\Gamma_k c_{\sigma}^\dagger \alpha_{k\sigma} + \text{H.c.} \right). \quad (11)$$

with the self-consistency equation

$$\Delta(\omega) = \sum_{\vec{k}} \frac{|\Gamma_{\vec{k}}|^2}{\omega - E_{\vec{k}}} = \frac{W^2}{4} \mathcal{G}_c(\omega). \quad (12)$$

Equation (12) is valid for a semi-elliptic density of states of the conduction electrons

$$\rho_0(\epsilon) = \frac{2}{\pi W^2} \sqrt{W^2 - \epsilon^2}. \quad (13)$$

In all our calculations we choose $W = 1$ as unit of energy.

In order to solve numerically the impurity model (9) we make use of the resolvent perturbation theory introduced in Ref. 21. It serves as a basis for the non-crossing approximation to the Anderson impurity model²⁵ which has been successfully extended to investigate the finite- U Anderson impurity model,²⁶ the Emery model in the dynamical mean field theory,²⁷ and the Anderson-Hubbard model in this approximation.¹⁵ As described in Ref. 15, the occurring coupled integral equations are solved numerically by introducing defect propagators²⁸ and making use of the fast Fourier transformation.²⁷

III. RELATION WITH THE ANDERSON-HUBBARD MODEL

It is well known that the Anderson and Kondo impurity model are mutually related,¹⁸ as well as the lattice models.^{19,20} We expect that also the lattice models which include interactions among the conduction electrons show the same low-energy behavior. Within the dynamical mean-field theory this should be true provided the excitation energies of the corresponding impurities are the same in both models. In Ref. 15 we have derived the effective impurity model $H_{\text{A,imp}} = H_{\text{med}} + H_{\text{loc}}$ for the Anderson-Hubbard model. The local part reads

$$H_{\text{loc}} = -\frac{1}{2}U_c \sum_{\sigma} c_{\sigma}^\dagger c_{\sigma} + U_c n_{\uparrow}^c n_{\downarrow}^c + V \sum_{\sigma} (c_{\sigma}^\dagger f_{\sigma} + \text{H.c.}) - \frac{1}{2}U_f \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma} + U_f n_{\uparrow}^f n_{\downarrow}^f. \quad (14)$$

Note that the mapping being discussed here is based on the impurity models and not on the original lattice models. Therefore, the same restrictions apply as to the dynamical mean-field theory or the limit of infinite coordination number of the underlying lattice. In particular, spatial correlations are not included, so that an RKKY interaction will not occur,²⁹ in contrast to the treatment in finite dimensions.²⁰

It has been found in Ref. 15 that two characteristic features occur at low energies for the Anderson-Hubbard model. At intermediate temperatures, a quasiparticle peak is formed at the chemical potential which corresponds to the quasiparticle peak observed for a pure Hubbard model.^{23,30,31} In this temperature regime the presence of the f orbitals does not influence the low-energy behavior. When lowering the temperature a gap opens. As in the case of free conduction electrons, this is interpreted as a hybridization gap which arises from the level crossing of the quasiparticle band with dynamically created states at the chemical potential (Kondo-resonance states).^{32,29}

Both features are related to transition energies of the impurity which generate a Kondo effect on a certain energy scale when coupled to a bath. The eigenenergies of the impurity (14) where the f orbital is singly occupied when $V \rightarrow 0$ are listed in Tab. I. The Hubbard-like quasiparticle peak is not influenced by the presence of the f orbitals and results therefore from the c charge degree of freedom. The relevant transition in H_{loc} is $f^1 c^0 \rightarrow f^1 c^1(S)$ (S stands for singlet) with its energy given by $\Delta E_1 = E(f^1 c^0) - E(f^1 c^1(S))$. The opening of the gap is found at lower temperatures and it is related to the singlet-triplet excitation $f^1 c^1(T) \rightarrow f^1 c^1(S)$ (the lowest transition energy of the impurity) with energy $\Delta E_2 = E(f^1 c^1(T)) - E(f^1 c^1(S))$.

The two impurity models generate the same low-energy behavior, provided their corresponding low-energy transitions have identical energies. The eigenenergies of

	AHM	KHM
$E(f^1 c^0)$	$-\frac{U_f + U_c}{4} - \frac{1}{4}\sqrt{(U_f - U_c)^2 + 16V^2}$	0
$E(f^1 c^1(S))$	$-\frac{U_f + U_c}{4} - \frac{1}{4}\sqrt{(U_f + U_c)^2 + 64V^2}$	$-\frac{U_c}{2} - \frac{3J}{4}$
$E(f^1 c^1(T))$	$-\frac{U_f + U_c}{2}$	$-\frac{U_c}{2} + \frac{J}{4}$
$E(f^1 c^2)$	$-\frac{U_f + U_c}{4} + \frac{1}{4}\sqrt{(U_f - U_c)^2 + 16V^2}$	0

TABLE I. Eigenenergies of the impurity, H_{loc} , in the Anderson- (AHM) and Kondo-Hubbard model (KHM) in the symmetric case. The indicated occupation is the one for $V \rightarrow 0$. $S(T)$ stands for singlett (triplett) configuration, resp. States not included for the AHM have zero f occupation in the limit $V \rightarrow 0$ and no counterpart in the KHM.

the Kondo impurity (10) are listed in Tab. I as well. We determine the parameters of the Kondo-Hubbard model by equating the corresponding transition energies. The exchange coupling constant J is obtained from $E(f^1 c^1(T)) - E(f^1 c^1(S)) = \Delta E_2 = J$

$$J = \frac{1}{4}\sqrt{(U_f + U_c)^2 + 64V^2} - \frac{1}{4}(U_f + U_c) = \frac{8V^2}{U_f + U_c} + o(V^4). \quad (15)$$

The Hubbard interaction in the Kondo-Hubbard model, which we denote by \tilde{U}_c in order to distinguish it from the Anderson-Hubbard model, is obtained from $E(f^1 c^0) - E(f^1 c^1(S)) = \Delta E_1 = \tilde{U}_c/2 + 3/4J$

$$\begin{aligned} \tilde{U}_c &= \frac{3}{8}(U_f + U_c) - \frac{1}{2}\sqrt{(U_f - U_c)^2 + 16V^2} \\ &\quad + \frac{1}{8}\sqrt{(U_f + U_c)^2 + 64V^2} \\ &= U_c \left(1 - \frac{8V^2}{U_f^2 - U_c^2}\right) + o(V^4). \end{aligned} \quad (16)$$

Whereas the appearance of the exchange coupling J as well as its magnitude for small V is expected (the intermediate state requires a doubly occupied c orbital with energy $U_c/2$), the modification of the local interaction of the conduction electrons might be surprising. However, if f charge fluctuations are possible, a doubly occupied c orbital may lower its energy by virtual transitions onto the f orbital. To compensate, the effective repulsion is lowered when the f occupancy is fixed.

The same relations between the parameters of the Anderson- and Kondo-Hubbard model are obtained by performing a canonical transformation of the molecule where one eliminates the charge degrees of freedom of the f orbital in perturbation theory in the hybridization V . This is shown in App. A.

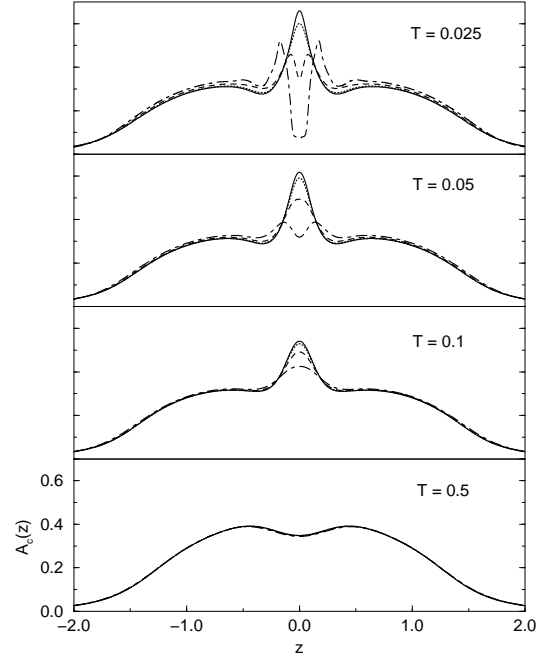


FIG. 1. Local density of states $A_c(z)$ in the Kondo-Hubbard model for $U_c = 1$ and $J = 0$ (solid), 0.05 (dotted), 0.1 (dashed), and 0.15 (dot-dashed line) at different temperatures.

IV. RESULTS

In Fig. 1 we display the local spectral functions of the conduction electrons which were obtained by the treatment outlined in Sec. II for $U_c = 1$ and various J at different temperatures T . The results found are typical for the Kondo-Hubbard model. At comparatively high temperatures ($T > 0.5$), only two broad maxima are seen which correspond to upper and lower Hubbard band of the conduction electrons. When lowering the temperature, a peak emerges at the chemical potential. The spectra at these temperatures are almost independent of the coupling J to the f spin for small $J \lesssim 0.1$, and coincide with the spectra calculated for the pure Hubbard model ($J = 0$). Therefore, we attribute this peak to the quasiparticle peak of the Hubbard model^{30,31,33} which describes the conduction electrons. At these moderate temperatures the c and f electrons are almost decoupled. The quasiparticle peak corresponds to the $c^1 \rightarrow c^0$ transition in the c - f molecule. Coupled to the bath, this transition gives rise to a Kondo effect, which sets a characteristic energy scale. Assuming $J = 0$ and a structureless bath with $\Delta(0) = 2/\pi$, the impurity model reduces to the symmetric Anderson model and the Kondo temperature is estimated to $T_K \sim 0.5$.³⁴ (This rather large

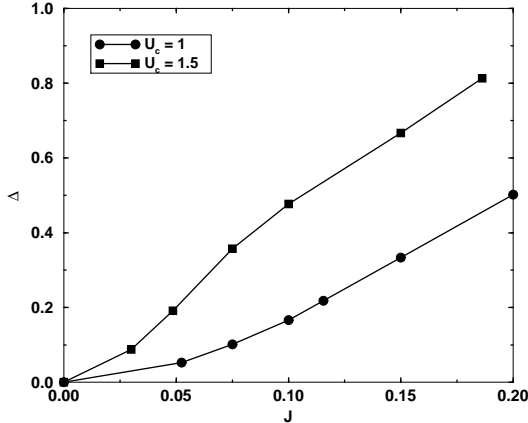


FIG. 2. Gaps of the Kondo-Hubbard model for $U_c = 1.0$ and 1.5 . The lines are guides to the eye.

scale is due to the large coupling of the impurity to the bath which is of the order of the band-width D .) Notice that the given value of T_K provides only a rough estimation of the corresponding energy scale in our calculation. First of all, the assumption of a structureless Δ is not valid. Moreover, neglecting vertex corrections in the NCA for the symmetric Anderson model, as we have done, underestimates the Kondo temperature.²⁶

When we reduce the temperature further, we observe that the quasiparticle peak gets split (Figs. 1). This splitting results from the influence of the f spins since its characteristic temperature, as well as its magnitude depend on J . Therefore, the f and c subsystems are no longer decoupled in this temperature regime. At the lowest temperatures that we reach numerically, and which are lower when J becomes smaller, a gap begins to open as is expected for the symmetric model. Qualitatively, these findings fit to the scenario encountered in the Anderson model with free conduction electrons, where below a characteristic temperature a local Kondo effect takes place, in which the conduction electrons screen the f spin, which leads to a resonance at the chemical potential in the particle-hole symmetric case. These dynamically generated states cross the conduction-band states, one finds a splitting of the conduction band with a gap at the chemical potential, and the system becomes an insulator.^{32,29,16}

Quantitatively, however, these effects depend not only on the exchange interaction J but also on the local Hubbard interaction of the conduction electrons U_c . This is seen in Fig. 2 where we plot the gaps measured as the distance between the two maxima for $U_c = 1$ and 1.5 vs. J . As discussed for the Anderson-Hubbard model,¹⁵ our numerical procedure does not allow to proceed to very low temperatures. As the gaps have not yet completely converged we only repeat the following qualitative remark which applied also for the Anderson-Hubbard model: The larger U_c , the larger the resulting gap, and as

in the case of the Anderson-Hubbard model, the quasi-particles of the Hubbard model are responsible for the screening of the f moment.

Next, we compare these findings to the results of the Anderson-Hubbard model¹⁵ in Fig. 3 (left). The parameters of the Kondo-Hubbard model, $U_c = 1.479$ and $J = 0.04851$, were chosen such that the model originates from an Anderson-Hubbard model with $U_c = 1.5$, $U_f = 5$, and $V = 0.2$ — see Sec. III. The most obvious difference is the presence of the f peak at $z \sim \pm U_f/2$ in the latter case which corresponds to the possible charge fluctuation on the f orbital. Except for this, we find that the two spectra are similar. Since the Kondo-Hubbard model was derived from the Anderson-Hubbard model by projecting out charge fluctuations on the f orbital this should be expected for a small hybridization V where these charge fluctuations are unimportant.

However, close to the chemical potential the two spectra only qualitatively agree. This should not be too surprising, as in the canonical transformation the one-particle operators should be transformed as well in order to obtain equivalent spectra,³⁵ see also App. A. Besides higher Green's functions, one finds contributions from \mathcal{G}_{cf} and \mathcal{G}_f of the Anderson-Hubbard model to the c spectral function of the Kondo-Hubbard model. We end this section by reporting a strange observation. If we ignore the change of U_c when passing from the Anderson-Hubbard model to the Kondo-Hubbard model, a difference between the two spectra can hardly be seen at small V , Fig. 3 (right). The rather strong influence of U_c on the spectra (U_c changed by 1.4% from Fig. 3 (left) to Fig. 3 (right)) is due to the proximity to the metal-insulator of the bare conduction electrons which in our scheme occurs at $U_c \sim 1.7$. For larger values of V this finding does not hold true, but the agreement in total gets worse since charge fluctuations become more important.

V. CONCLUSIONS

In summary, we investigated a Kondo lattice model with correlated conduction electrons within the dynamical mean-field theory. To this end we mapped the model onto an impurity model in which a unit cell of the lattice is embedded self-consistently into a bath of free electrons. This impurity model was studied numerically within the resolvent perturbation theory by applying the non-crossing approximation.

The parameters of the Kondo-Hubbard model were related to the parameters of the Anderson-Hubbard model by matching the transition energies within a single unit cell. It was shown that this is equivalent to performing a canonical transformation within a single unit cell.

The resulting spectral functions (local density of states) behave similarly as in the Anderson-Hubbard model: At relatively high temperatures the conduction electrons are almost decoupled from the f electrons and,

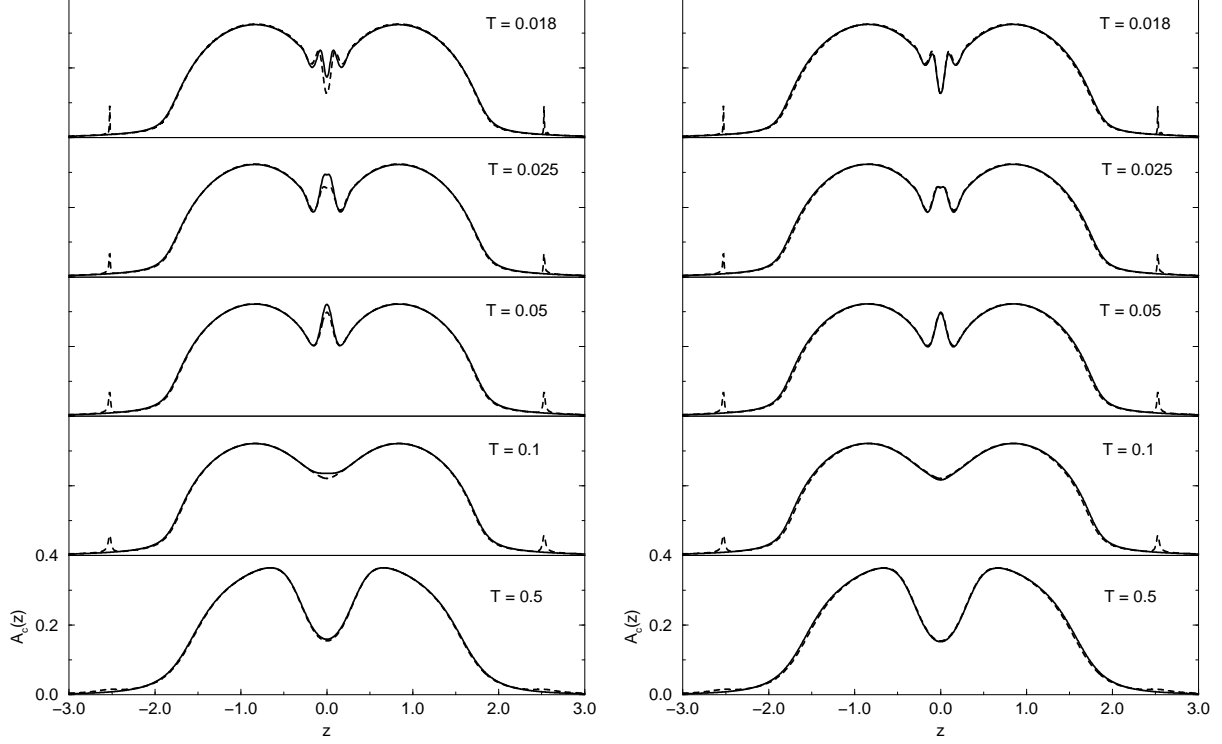


FIG. 3. Local density of states $A_c(z)$ in the Kondo-Hubbard model (solid lines, $J = 0.04851$, $U_c = 1.479$, left, and $U_c = 1.5$, right) and the Anderson-Hubbard model (dashed lines, $U_c = 1.5$, $U_f = 5$, $V = 0.2$) at different temperatures.

as in the pure Hubbard model, we observe a quasiparticle peak emerging when the temperature is lowered. When the temperatures is reduced further, the quasiparticle peak splits and a gap opens. As in the case of free conduction electrons, one might envisage that a (local) Kondo effect generates resonances at the chemical potential which hybridize with the quasiparticle states leading to a gap.

The correlations among the conduction electrons, however, do not only show up in the formation of a quasiparticle peak at high temperatures, but also influence the size of the gap at low temperatures. In agreement with the Anderson-Hubbard model, we find that the low-energy scale is increased as the correlations become stronger.

Both features result from certain transitions in the impurity model. The first one, which corresponds to the Hubbard quasiparticle peak, is related to the (local) transition where the c orbital changes from single to double (empty) occupancy, whereas the second one, leading to the gap, stems from the singlet-triplet transition of the c - f molecule which has a lower energy. The considered impurity model is a “minimal” model which contains two different excitation energies and the Kondo-Hubbard model is a minimal model to generate the two features mentioned above. Therefore it deserves continued interest.

APPENDIX A: CANONICAL TRANSFORMATION

The traditional way of deriving Kondo models from Anderson models is to perform a canonical transformation

$$H_K = e^S H_A e^{-S} \quad (A1)$$

such that there is no c - f hybridization in H_K and the f occupancy is conserved.¹⁸ Usually this is done in perturbation theory with respect to the c - f hybridization V . We will perform this transformation on the level of the impurity models and rewrite our impurity model as

$$H_{A,\text{imp}} = H_0 + H_1, \quad (A2)$$

$$H_0 = H_\alpha + H_{\alpha c} + H_c + H_f, \quad (A3)$$

$$H_1 = H_{cf}. \quad (A4)$$

The transformed Hamiltonian is given by

$$H_{K,\text{imp}} = e^S H_{A,\text{imp}} e^{-S} = e^S H_{A,\text{imp}} \quad (A5)$$

$$\begin{aligned} &= H_0 + H_1 + \mathcal{S}_1 H_0 + \frac{1}{2} \mathcal{S}_1^2 H_0 + \mathcal{S}_1 H_1 \\ &\quad + \mathcal{S}_3 H_0 + \frac{1}{2} \mathcal{S}_1^2 H_1 + \frac{1}{6} \mathcal{S}_1^3 H_0 + \mathcal{S}_3 H_1 + \mathcal{S}_3 \mathcal{S}_1 H_0 \\ &\quad + \frac{1}{6} \mathcal{S}_1^3 H_1 + \frac{1}{24} \mathcal{S}_1^4 H_0 + o(V^5) \end{aligned} \quad (A6)$$

where $\mathcal{S}A = [S, A]_-$ and $\mathcal{S}_\nu \sim V^\nu$. Charge fluctuations on the f orbital are eliminated by choosing \mathcal{S} such that there are no contributions of odd power in V . Hence,

$$\mathcal{S}_1 H_0 = -H_1 \Rightarrow S_1 = \frac{1}{\mathcal{L}_0} H_1, \quad (\text{A7})$$

$$\mathcal{S}_3 H_0 = -\frac{1}{3} \mathcal{S}_1^2 H_1 \Rightarrow S_3 = \frac{1}{3} \frac{1}{\mathcal{L}_0} \mathcal{S}_1^2 H_1. \quad (\text{A8})$$

where the Liouvillean \mathcal{L}_0 is defined by $\mathcal{L}_0 A = [H_0, A]_-$. The effective Hamiltonian which conserves the f occupation is then given by

$$H_{K,\text{imp}} = H_0 + \frac{1}{2} \mathcal{S}_1 H_1 + \frac{1}{8} \mathcal{S}_1^3 H_1. \quad (\text{A9})$$

In order to reproduce the previous results from Sec. III we will neglect $H_{\alpha c}$ and thus replace \mathcal{L}_0 in Eqs. (A8) by $\mathcal{L}_c + \mathcal{L}_f$. The Liouvillean is easily inverted by decomposing $c_\sigma^\dagger = \hat{c}_\sigma^\dagger + \bar{c}_\sigma^\dagger$ where

$$\hat{c}_\sigma^\dagger = c_\sigma^\dagger (1 - n_{-\sigma}^c), \quad \bar{c}_\sigma^\dagger = c_\sigma^\dagger n_{-\sigma}^c \quad (\text{A10})$$

are eigenoperators of \mathcal{L}_c with eigenvalues $-U_c/2$ and $U_c/2$, resp. (similarly for f_σ^\dagger). We immediately obtain S_1 and find as effective Hamiltonian within the space $n_f = 1$:

$$H_{K,\text{imp}} = H_\alpha + H_{\alpha c} + H_c \quad (\text{A11})$$

$$+ JS_f S_c + \delta U_c \left(-\frac{1}{2} n^c + n_\uparrow^c n_\downarrow^c \right), \quad (\text{A12})$$

where we dropped a constant and

$$J = \frac{8V^2}{U_f + U_c} - \frac{128V^4}{(U_f + U_c)^3}, \quad (\text{A13})$$

$$\begin{aligned} \delta U_c = & -4V^2 \left(\frac{1}{U_f - U_c} - \frac{1}{U_f + U_c} \right) \\ & + 16V^4 \left(\frac{1}{(U_f - U_c)^3} - \frac{4}{(U_f + U_c)^3} \right). \end{aligned} \quad (\text{A14})$$

These are just the results (15) and (16) found in the previous section by comparing the excitation energies of the impurity in both models.

Note that we neglected the coupling of the c - f molecule to the bath in this derivation. In reality the α operators should change in the canonical transformation as well. This approximation corresponds to just matching the molecular excitation energies in the previous section. Note also that the canonical transformation was performed on the impurity model. Therefore no RKKY interaction is generated to forth order in V .

When comparing spectral functions of models related by canonical transformations one should bear in mind that the creation operators should be transformed as well.³⁵ This is seen as follows: The Hamiltonians in both models are related by (A5), the ground states via

$$|\Psi_K\rangle = e^S |\Psi_A\rangle. \quad (\text{A15})$$

Thus, the c correlation function, e.g., of the Kondo-Hubbard model is given by

$$\begin{aligned} \mathcal{C}_K(z) &= \left\langle \Psi_K \left| c_\sigma \frac{1}{z - H_K} c_\sigma^\dagger \right| \Psi_K \right\rangle \\ &= \left\langle \Psi_A \left| (e^S)^\dagger c_\sigma (e^{-S})^\dagger \frac{1}{z - H_A} e^{-S} c_\sigma^\dagger e^S \right| \Psi_A \right\rangle \end{aligned} \quad (\text{A16})$$

(and correspondingly the Green's function). In particular, the c Green's function in the Kondo-Hubbard model is not identical to the one in the Anderson-Hubbard model. Given S_1 we find to first order

$$\begin{aligned} e^{-S} c_\sigma^\dagger e^S &= c_\sigma^\dagger + 2V \left\{ \frac{2U_c}{U_f^2 - U_c^2} \times \right. \\ &\quad \left(-c_\sigma^\dagger c_{-\sigma}^\dagger f_{-\sigma} + c_\sigma^\dagger f_{-\sigma}^\dagger c_{-\sigma} + f_\sigma^\dagger c_{-\sigma}^\dagger c_{-\sigma} \right) \\ &\quad \left. - \frac{1}{U_f - U_c} \hat{f}_\sigma^\dagger + \frac{1}{U_f + U_c} \bar{f}_\sigma^\dagger \right\}. \end{aligned} \quad (\text{A17})$$

APPENDIX: ACKNOWLEDGMENTS

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